

MOLECULAR PROCESSES IN COMETS

Grant NAGW-1561

Final Report

For the period 1 January 1989 through 31 October 1997

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January 1998

Prepared for  
National Aeronautics and Space Administration  
Washington, D. C. 20546

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The Smithsonian Astrophysical Observatory  
is a member of the  
Harvard-Smithsonian Center for Astrophysics

The NASA Technical Officer for this grant is Dr. Jay Bergstralh, Code EL,  
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FINAL

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The research focused on molecular hydrogen and its response to ultraviolet radiation, photoelectron impact excitation and X-ray radiation and on the interpretation of the ultraviolet spectra of the Jupiter dayglow and auroras.

A systematic effort was made to obtain reliable rate coefficients for rovibrational energy transfer of  $H_2$ , particularly in collisions with hydrogen atoms.

We carried out elaborate quantum-mechanical calculations of the scattering of H and  $H_2$  on what had been characterized as a reliable potential energy surface of the  $H_3$  molecular system (Sun and Dalgarno 1994). These calculations took into account reactive channels and rate coefficients for ortho-para transitions were obtained.

Quantal calculations are too complex to be applied to all the possible rovibrational transitions and we turned to a semi-classical method. With it we calculated rate coefficients for transitions, reactive and non-reactive, for all the rovibrational levels (Lepp, Buch and Dalgarno 1995). We carried out the calculations for three of the available  $H_3$  potential energy surfaces. We discovered an unexpected sensitivity of the rate coefficients for the non-reactive channels to the potential energy surface. This discovery stimulated more thorough investigations of the potential energy surface elsewhere and to the construction of a new surface. We have used it in further semi-classical calculations in work that will shortly be

completed and which, together with new quantum-mechanical calculations should comprise a set of reliable rate coefficients that can be used in discussions of  $\text{H}_2$  on the Jovian planets.

We carried out a detailed study of the Jovian ultraviolet dayglow. There has been a long-running argument about the dayglow on Jupiter. There are two sources of excitation: fluorescence and photoelectron impact excitation. It had been argued that a third source “the electron glow” was needed to bring theory and observation into agreement. We believe we have shown conclusively that the third source is unnecessary. We have achieved a close quantitative agreement between the predicted spectrum arising from fluorescence and photoelectrons and the measured spectrum (Liu and Dalgarno 1996a). We also demonstrated a method by which the presence of HD could be established observationally.

Similar calculations were carried out of the ultraviolet spectra of the Jovian auroras (Liu and Dalgarno 1996b). We again found close agreement. Indeed, the agreement was so detailed we were able to derive the temperature of the atmosphere. We found, contrary to the standard model of the time, a high temperature between 400K and 600K and established the presence of a significant temperature gradient. A large temperature gradient was indeed found by direct sampling with the Jupiter probe.

With the collisional data we had acquired, we studied the response of a gas of molecular hydrogen to incident X-ray radiation (Tin   et al 1997) but we have yet to apply the results to the planets.

### References

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